

**CROSS SECTIONS FOR ELECTRON IMPACT EXCITATION OF IONS  
RELEVANT TO PLANETARY ATMOSPHERES OBSERVATION**

1N-91  
337 467

**FINAL REPORT**

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**PERIOD**

April 1, 1995 - June 30, 1998

Prepared for the National Aeronautics and Space Administration  
**PLANETARY ATMOSPHERES PROGRAM**  
Solar System Exploration Division  
Office of Space Science  
**NASA HEAD QUARTER GRANT: NAGW-4447**  
**NASA GSFC GRANT: NAG5-4763**

The goal of this research grant was to calculate accurate oscillator strengths and electron collisional excitation strengths for inelastic transitions in atomic species of relevance to Planetary Atmospheres. Large scale configuration-interaction atomic structure calculations have been performed to obtain oscillator strengths and transition probabilities for transitions among the fine-structure levels and R-matrix method has been used in the calculations of electron-ion collision cross sections of C II, S I, S II, S III, and Ar II. A number of strong features due to ions of sulfur have been detected in the spectra of Jupiter satellite Io. The electron excitation cross sections for the C II and S II transitions are studied in collaboration with the experimental atomic physics group at the Jet Propulsion Laboratory. There is excellent agreement between experiment and theory which provide an accurate and broad-base test of the ability of theoretical methods used in the calculation of atomic processes. Specifically, following research problems have been investigated:

#### 1. Electron Impact Excitation Cross Sections of C II.

Electron collisional excitation cross sections were calculated for inelastic transitions in C II from the ground state  $2s^2 2p^2 P^0$  to the excited states  $2s 2p^4 4P$ ,  $2D$ , and  $2S$  at wavelengths 2324 Å, 1335 Å, and 1036 Å, respectively by including the LS states  $2s^2 2p^2 P^0$ ,  $2s 2p^4 4P$ ,  $2D$ ,  $2S$ ,  $2P$ ,  $2s^2 3s^2 S$ ,  $2s^2 3p^2 P^0$ , and  $2p^3 4S^0$  in the close-coupling expansion [1]. There is excellent agreement between theory and experiment.

#### 2. Electron Impact Excitation Cross Sections of S III.

Electron collisional excitation strengths for all electric dipole allowed, intercombination, and forbidden transitions among the lowest 17 LS states  $3s^2 3p^2 3P$ ,  $1D$ ,  $1S$ ,  $3s 3p^3 5S^0$ ,  $3D^0$ ,  $3P^0$ ,  $1P^0$ ,  $3S^0$ ,  $1D^0$ ,  $3s^2 3p 3d 1D^0$ ,  $3F^0$ ,  $3P^0$ ,  $3D^0$ ,  $1F^0$ ,  $1P^0$ , and  $3s^2 3p 4s 3P^0$ ,  $1P^0$  of S III are calculated using the R-matrix method [2]. These states are represented by extensive configuration-interaction wave functions that yield excited states energies in close agreement with recent laboratory measurements. The effective collision strengths are determined over a wide-temperature range assuming a Maxwellian distribution of electron energies.

#### 3. Energy Levels and Oscillator Strengths for Transitions in S III.

Accurate values of oscillator strengths and transition probabilities for transitions between the multiplets of the  $3s^2 3p^2$ ,  $3s 3p^3$ ,  $3s^2 3p 3d$ ,  $3s^2 3p 4s$ ,  $3s^2 3p 4p$ , and  $3s^2 3p 4d$  configurations of S III are calculated using extensive configuration-interaction wave functions [3]. The LS states belonging to these configurations give rise to 53 fine-structure levels when relativistic effects are considered. We have calculated oscillator strengths and transition probabilities for all dipole-allowed and intercombination transitions between these 53 fine-structure levels [4]. The relativistic effects in intermediate coupling scheme are included in the Breit-Pauli formulaion.

#### 4. Collision Strengths for Electron Collisional Excitation of S II.

This research has been completed in collaboration with the JPL experimental atomic physics group [5]. The calculated cross sections show excellent agreement with the

energy-loss, merged-beams measurements at JPL for all three transitions  $3s^2 3p^3 \ 4S^0 - 3s^2 3p^3 \ 2D^0, 2P^0$ , and  $3s 3p^4 \ 4P$  in S II at wavelengths 6716 Å, 4069 Å, and 1256 Å, respectively.

Electron collision excitation strengths for 171 inelastic transitions in S II are calculated in a 19-state ( $3s^2 3p^3 \ 4S^0, 2D^0, 2P^0, 3s 3p^4 \ 4P, 2D, 2S, 3s^2 3p^2 3d \ 2P, 4F, 4D, 2F, 4P, 3s^2 3p^2 4s \ 4P, 2P, 3s^2 3p^2 4p \ 2S^0, 4D^0, 2D^0, 4S^0, 2P^0$ ) close-coupling approximation [6]. Rydberg series of resonances converging to the excited states are explicitly included in the collision strengths.

## 5. Electron Impact Excitation of Inelastic Transitions in Ar II.

Collision Strengths for electron impact excitation of inelastic transitions in Ar II were calculated in two independent nine- and nineteen-state close-coupling approximations. The effective collision strengths have been calculated assuming a Maxwellian distribution of electron energies over a wide range of temperature [7].

## 6. Oscillator Strengths of Fine-Structure Transitions in Neutral Sulfur.

Oscillator Strengths and transition probabilities of electric-dipole-allowed and intercombination transitions from fine-structure levels of the ground  $3s^2 3p^4$  configuration to the levels belonging to configurations  $3p^3 4s, 3p^3 5s, 3p^3 3d$ , and  $3p^3 4d$  of neutral sulfur are calculated using extensive configuration-interaction wave functions [8].

## 7. Cross Sections for Inelastic Scattering of Electrons from Atomic Nitrogen.

The calculation of inelastic scattering of electrons from atomic nitrogen is performed by a graduate student as a part of his MS thesis research. Some of the preliminary results from this research were presented at the American Physical Society Meeting held in Santa Fe May 27-30, 1998.

## 8. Excitation of Atomic Ions by Electron Impact.

As a part of continuing worldwide effort to better understand electron-ion excitation processes for applications to astrophysical and laboratory plasmas, the best of a large body of atomic data available for carbon and oxygen ions have been evaluated, compiled, and recommended. This work has been published as a book chapter [9].

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**Students Supported:** Two graduate students, L. M. Richardson and C. A. Beatty, were partially supported by this grant. These students are working on their MS thesis research.

**Post-doctoral Research Associate:** Dr. G. P. Gupta, a postdoctoral researcher in the group was partially supported from this grant.